DOCUMENT RESUME

ED 267 738 IR 012 044

AUTHOR	Solomon, Sally; And Others
TITLE	The Drexel Chemistry Experience. Microcomputing Working Paper Series.
INSTITUTION	Drexel Univ., Philadelphia, PA. Microcomputing Program.
REPORT NO	MWPS-F-84-5
PUB DATE	May 85
NOTE	24p.
AVAILABLE FROM	Working Paper Series, Microcomputing Program, Office of the Vice President for Academic Affairs, Drexel University, Philadelphia, PA 19104.
PUB TYPE	Reports - Descriptive (141)
EDRS PRICE	MF01/PC01 Plus Postage.
DESCRIPTORS	*Chemistry; *Computer Assisted Instruction; *Computer Software; Higher Education; Instructional Materials; *Microcomputers; Program Descriptions; *Science Instruction; Teaching Methods
IDENTIFIERS	*Apple Macintosh; *Drexel University PA

ABSTRACT

The requirement that all Drexel University students purchase a Macintosh personal computer has had a strong impact on teaching methods throughout the university. The chemistry department now views the computer as a device that is ready to take its place beside other more traditional pedagogical tools. This document describes some of the numerous ways in which the Drexel chemistry department has contributed to the university-wide effort to develop computer-aided instructional materials. The software described includes an authoring system designed to create highly interactive tutorial lessons; other specialized materials allow the construction of molecular models, assignment of stereochemical designations, and study of the data and trends in an electronic periodic table. Chemistry department members' efforts to use the Macintosh in virtually every area of chemical education include laboratory, self-study, and simulation projects. For each project, the required hardware and software are mentioned, as well as the individuals primarily responsible for the concepts. (Author/THC)

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The Drexel Chemistry Experience

Sally Solomon, et al.
Department of Chemistry
Drexel University

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The Drexel Chemistry Experience

Introduction

The requirement that all Drexel University students purchase a Macintosh personal computer has had a strong impact on teaching methods throughout the university. In the chemistry department we now view the computer as a device that is ready to take its place beside the textbook, the chalkboard, the overhead projector, live demonstrations, study guides, homework assignments, problem-solving sessions and other more traditional pedagogical tools. Below is described the numerous ways in which the Drexel chemistry department has contributed to the university-wide effort to develop computer-aided instructional materials.

The use of computer-aided instruction in the chemistry department began before the first Macintosh arrived on campus, so this discussion is not limited to Macintosh applications. But when the Macintosh did get here, the attention of many chemistry department members was enthusiastically focused on ways to use the Macintosh in virtually every area of chemical education. The result of their efforts is summarized below where the field of chemical education is divided into several segments including lecture-presentation, laboratory, self-study and simulations. For each project we have mentioned the required hardware and software, as well as the individuals primarily responsible for the concepts. In a few cases computer applications were developed on the Lisa for "stand-alone" use on the Macintosh. Many more of the Macintosh projects have made use of available "generic" software packages including Macwrite (Apple) , Macpaint (Apple), Multiplan (Microsoft), TK! Solver (Software Arts/Lotus Development), and LessonWriter (developed at Drexel by Sally Solomon and Chris Nocella).

Computers in the Laboratory

Computers have already been applied in many chemistry laboratories at Drexel. More applications are being planned for future classes, in particular those to be attended by the first upperclassmen to have their own Macintoshes.

Prelab Videoquizzes (Apple IIe with Superpilot), A. Addison. One of the first uses of personal computers in the chemistry department was in the freshman general chemistry laboratory where it has been traditionally difficult to encourage students to read laboratory experiments before coming to class. The Drexel freshman chemistry laboratories are equipped with television monitors which are linked to an Apple IIe microcomputer in order to present timed quizzes. Specified time intervals and enlarged text were produced by using the Superpilot authoring system.

Video Messages (Apple IIe with Superpilot), D. Baer and S. Solomon. There are parts of each laboratory experiment in which special care must be taken to avoid errors or accidents. Sometimes students may not hear or remember the warnings given by their laboratory instructors. To highlight the "trouble spots" in an experiment we present colorful messages including graphics and animation designed to capture the attention of students before they have had a chance to go wrong (See Figure 1). We plan to incorporate the Macintosh into this project and are hopeful that the high-resolution graphics will more than compensate for the lack of color.

USE
Pipetting
Bulb
Not gour mouth

Figure 1. A Typical Laboratory Video Message

Prelab Drills (Mac with Lesson Writer²), S. Solomon and W. Kohlman. We are hoping to improve student performance in the laboratory and to help prevent accidents by providing interesting, game-like, computer-aided prelab lessons. The lessons were written using the LessonWriter² application. In each prelab lesson is a set of questions, most of which include diagrams of setups (See Figure 2a). Students can test themselves. At the end of each lesson they are asked to compare their score with that required to be ready for the laboratory class. In Figure 2b the final question in the lesson is shown, where you can see that the student user is not ready for the lab and is asked to repeat the lesson.

What do you throw away?
a) filtrate solution
b) solid in funnel

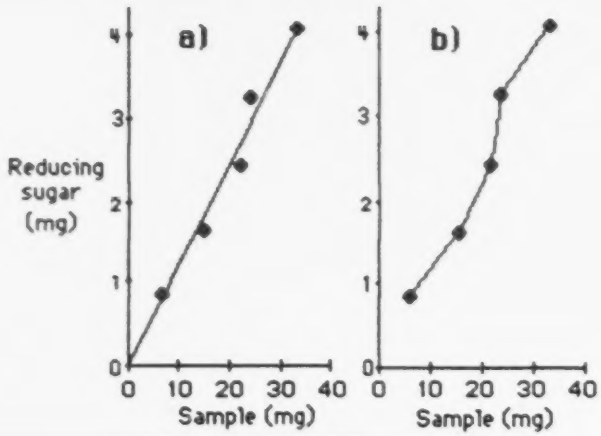
a

No! You just threw away your sample.

Figure 2a. Prelab Question (created with Lesson Writer)

File Edit Question Options Windows Lesson Help

Which of the figures shown looks most like your calibration plot?



a

Right. You should plot the best straight line. If your score is 9-12 you are ready to do this lab. If not quit, then repeat the lesson.

Try Again? Try Another? SCORE : 7 Quit

Figure 2b. Last Question in a Prelab Lesson

Taking Data (Mac with Microsoft Basic, 2.0). Fred Longo and Pat Nolan. We would like to introduce modern methods of data-taking in our upperclass laboratories. The use of the computer will allow our students to take data more efficiently and comprehensively. For instance, students will be able to follow the rates of very fast reactions (previously impractical) since there is virtually no time required to read and record data. The hardware needed to interface the physical chemistry laboratory instruments with the Macintosh is currently being developed in the Drexel chemistry department. Software is being designed that can be applied to a variety of different experiments, allowing data to be recorded at timed intervals.

Computers in Lecture

Drexel's chemistry lecture halls are equipped with Macintosh computers and projection equipment that expands the screen image so that it is visible to all.

Showing Figures (Mac with MacPaint). J. Friend. Lecturers prepare diagrams (formulas and apparatus) to illustrate points. The ability to move segments of the diagram around using the MacPaint lasso or "selector" makes this a particularly useful technique. For instance, the structures of carbohydrate molecules can be built up in this way. (See Figure 3).

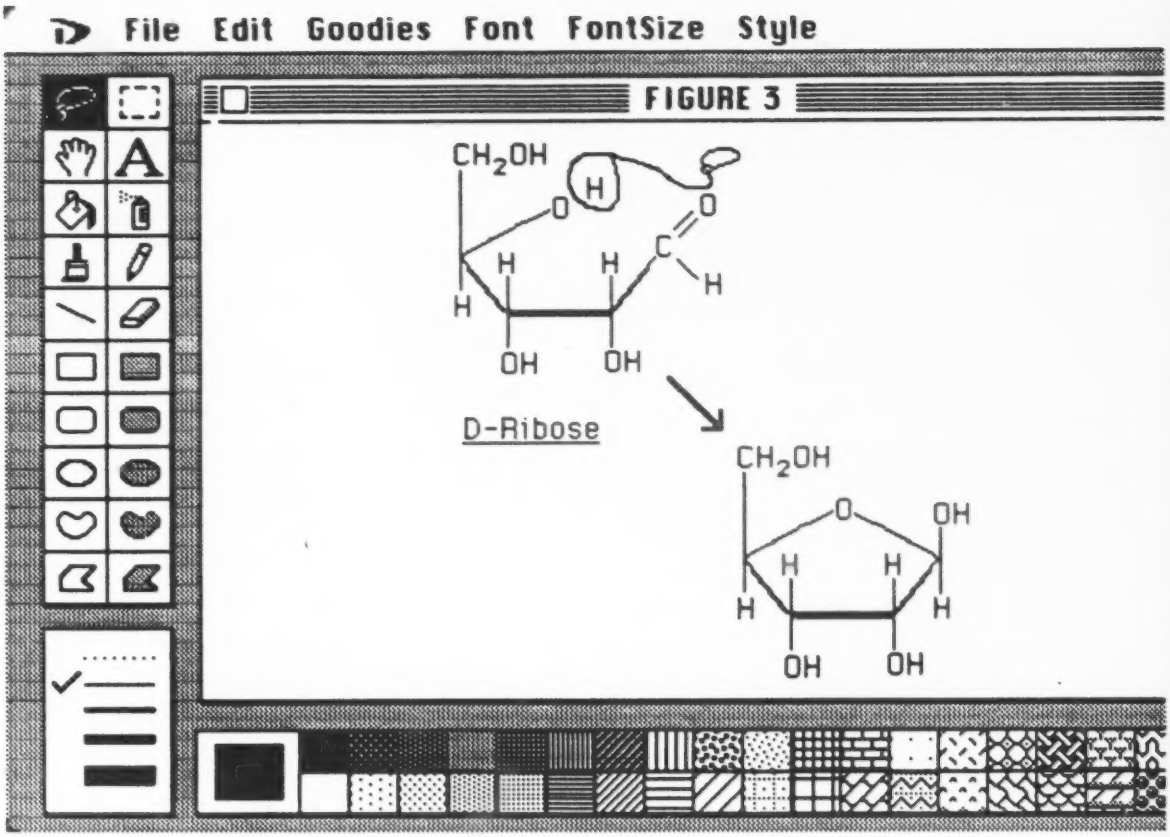


Figure 3. Formation of Cyclic Ribose

Equation Solving (Mac with TK! Solver), C. Rosenthal, A. Smith, S. Solomon. Equations (including quadratics and cubics) used to illustrate ideas are readily solved with the TK! Solver equation solving package. It is convenient to set up a single model and then to do repeated calculations to study it. For instance, students can see how well the van der Waals equation works in describing the behavior of a real gas (See Figure 4) and when approximations are allowed in calculations involving the ionization of weak acids and weak bases.

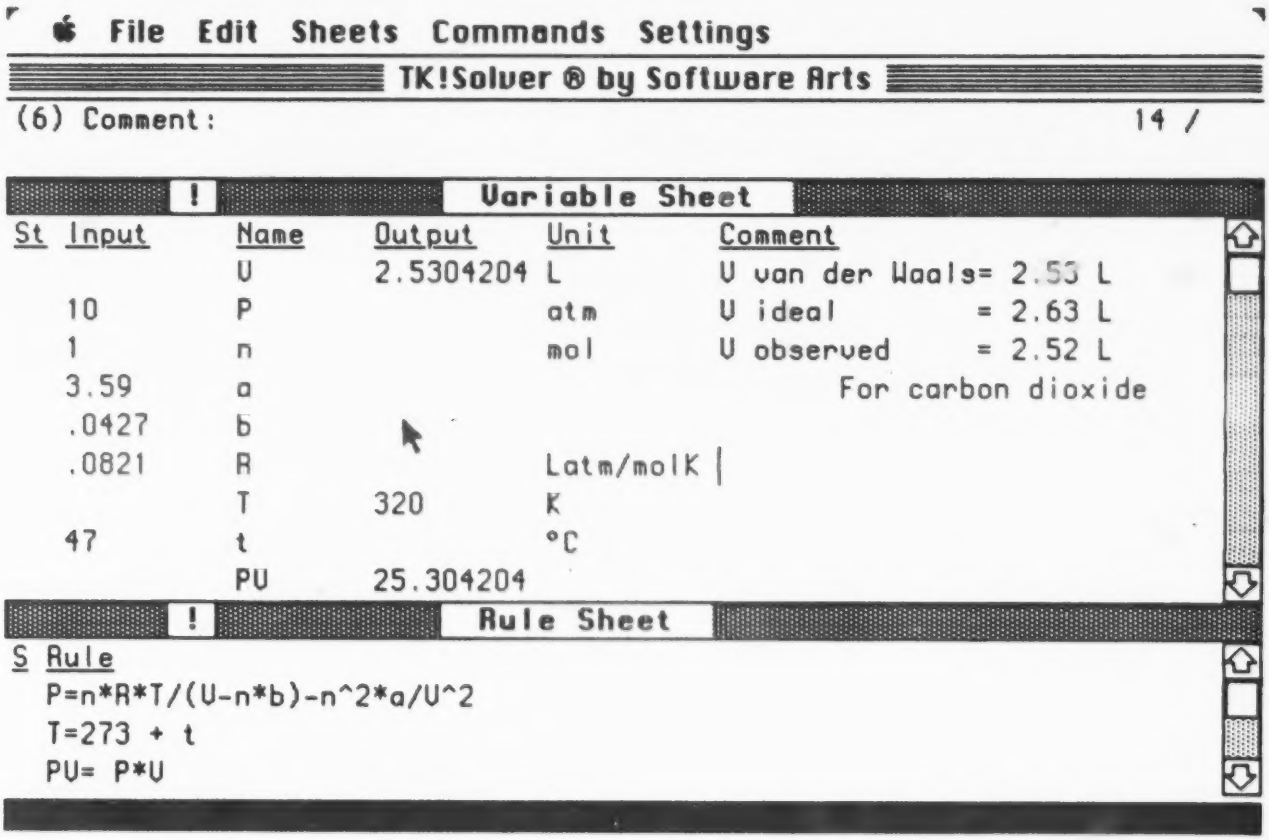


Figure 4. Solving the Van der Waals Equation

A number of TK! Solver models have been developed to solve problems involving concentrations of solutions, transition metal-ligand complex concentrations, acid-base titration curves, and the equilibrium chemistry of atmospheric cloud water. These have not yet been tested by students, but will soon become available in a text to be published by McGraw-Hill, entitled *Tk!Solver Pack in Chemical Equilibrium and Chemical Analysis* (Fall 1985) by Allan Smith.

Plotting (Mac with TK! Solver). C. Rosenthal. One area that is traditionally difficult for freshman chemistry students to comprehend is the meaning of an atomic orbital, a topic that is introduced in our introductory chemistry courses. The transition from mathematical equation to graphical representation is particularly baffling to students. To help them make this connection, the TK! Solver package is used to obtain orbital contour plots that arise from the functions that describe the electronic configuration of the hydrogen atom. Students are asked to participate in lecture by suggesting values for the contour; the resulting orbital shapes appear within a few seconds on the screen (See Figure 5). Using this method students can appreciate the differences between various kinds of orbitals. Using our normal lecture techniques students come away with an incomplete and rigid view of what an orbital is, since they see just *one* static version from *one* readymade diagram.

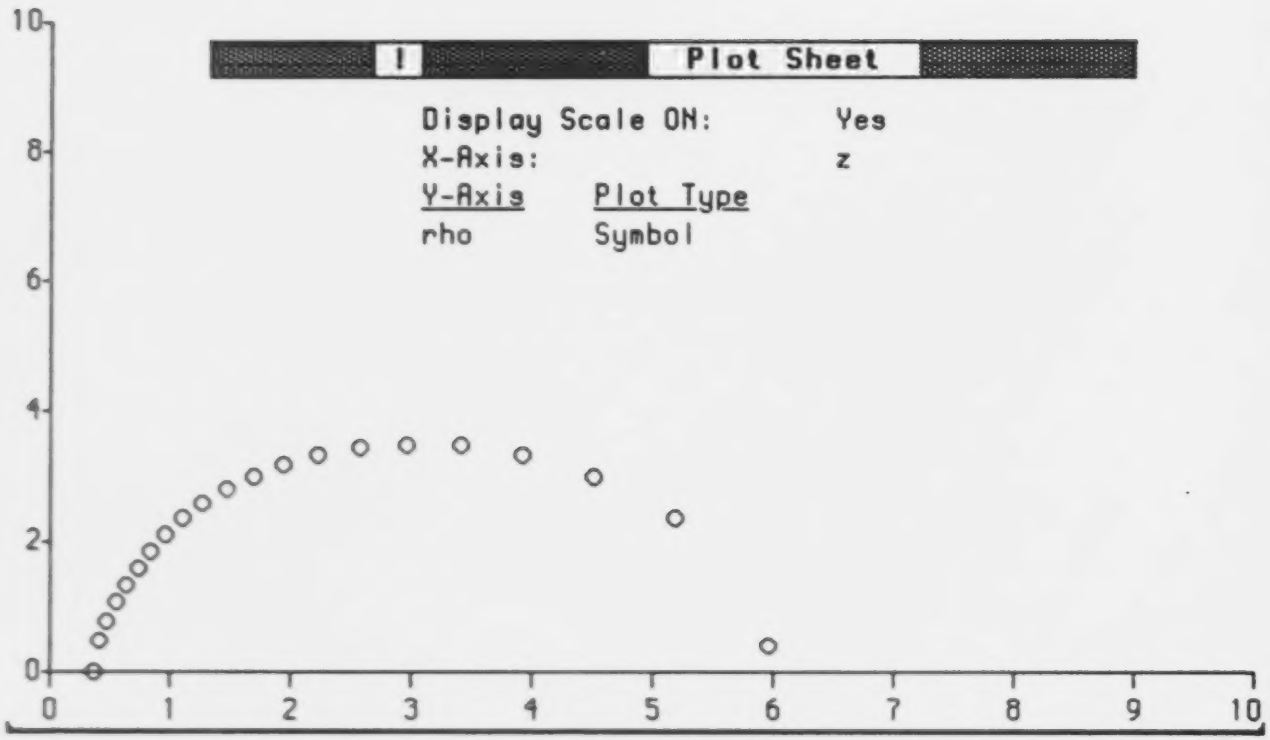


Figure 5. p_z Orbital Cross Section (with TKISolver)

Self Study

Many take home assignments are designed to make use of the Macintosh computer in Drexel chemistry courses.

Tutorials (Mac with Lesson Writer). The use of tutorial lessons is an established method that can be used to enhance skills in any area of education. Because it allows immediate feedback, the personal computer is an excellent vehicle for the administration of interactive lessons. In the Drexel chemistry department we have written chemistry lessons for beginning students in inorganic nomenclature, formula-writing, and organic nomenclature. By using the Lesson Writer application we can custom-design lessons to fit the material we present in our courses here at Drexel. Students asked to review the organic nomenclature lesson said that it was helpful and made the material easier to learn.

Chemical Calculations (Mac with Multiplan). A. Smith. Early in the first quarter of general chemistry students learn to calculate molecular weights and percentage compositions. We use this topic to familiarize students with the use of a spreadsheet in handling tables of data. The student enters a portion of the periodic table, as well as the formulas necessary to calculate molecular weights and percentage compositions.

Studying Equilibrium Systems (Mac with Multiplan). J. Friend and A. Smith. The study of equilibrium systems is normally very challenging for beginning chemistry students. To help them appreciate the nature of an equilibrium system we have provided models which the student can use to explore various systems. For instance, using a model describing a weak acid ionization, students were able to see how pH values depend upon concentrations of species present. Another model was demonstrated for plotting acid-base titration curves in which different concentrations of reactants could be entered by the student. To study a gaseous equilibrium system a problem set was handed out in which students were asked to solve for equilibrium concentrations of nitrogen, hydrogen, and ammonia in the Haber synthesis of ammonia, using a spreadsheet model provided for them.

Electronic Handbook of Chemistry (Mac with Peri-Chart). J. Friend. Easy access to a wide variety of tabulated data is contained in the application Peri-Chart. Normally students would need a chemical handbook and tables scattered throughout their texts in order to obtain the data available in Peri-Chart. For instance, a student wishing to learn about the properties of vanadium can, with a click of the mouse, see the material shown in Figure 6. In addition students can use Peri-Chart to test themselves on names, symbols, electronic configurations of elements as well as their positions in the periodic table. The application can also serve as a "chemical calculator" by supplying molecular weights when formulas are given. Properties of the elements can be compared to each other and can be plotted against atomic number to display interesting trends. We hope that Peri-Chart will encourage students to expand their chemical horizons by exploring data and trends beyond what is required for classroom assignments. Further, since the data are easily kept up-to-date, PeriChart should prove useful to advanced chemistry students and to professional scientists.

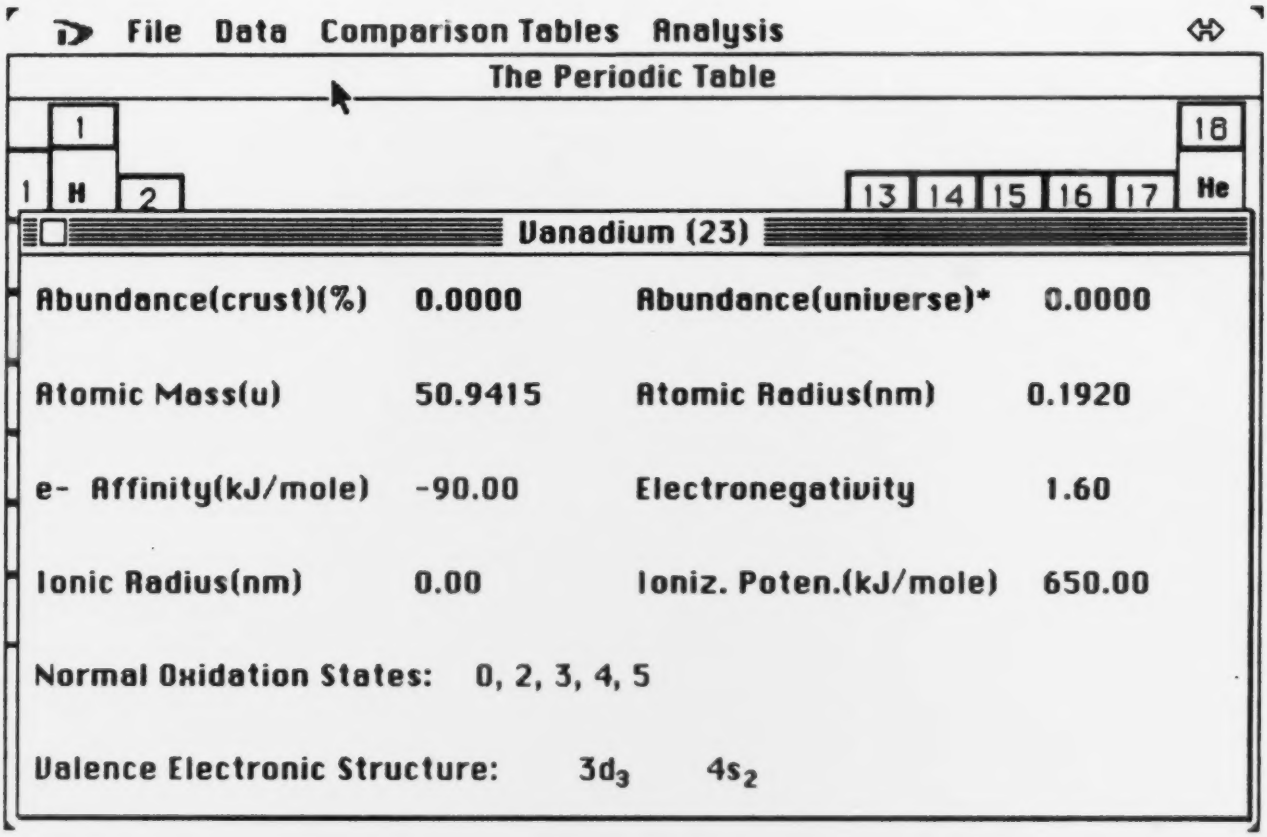


Fig. 6. Properties of Vanadium (From Peri-Chart)

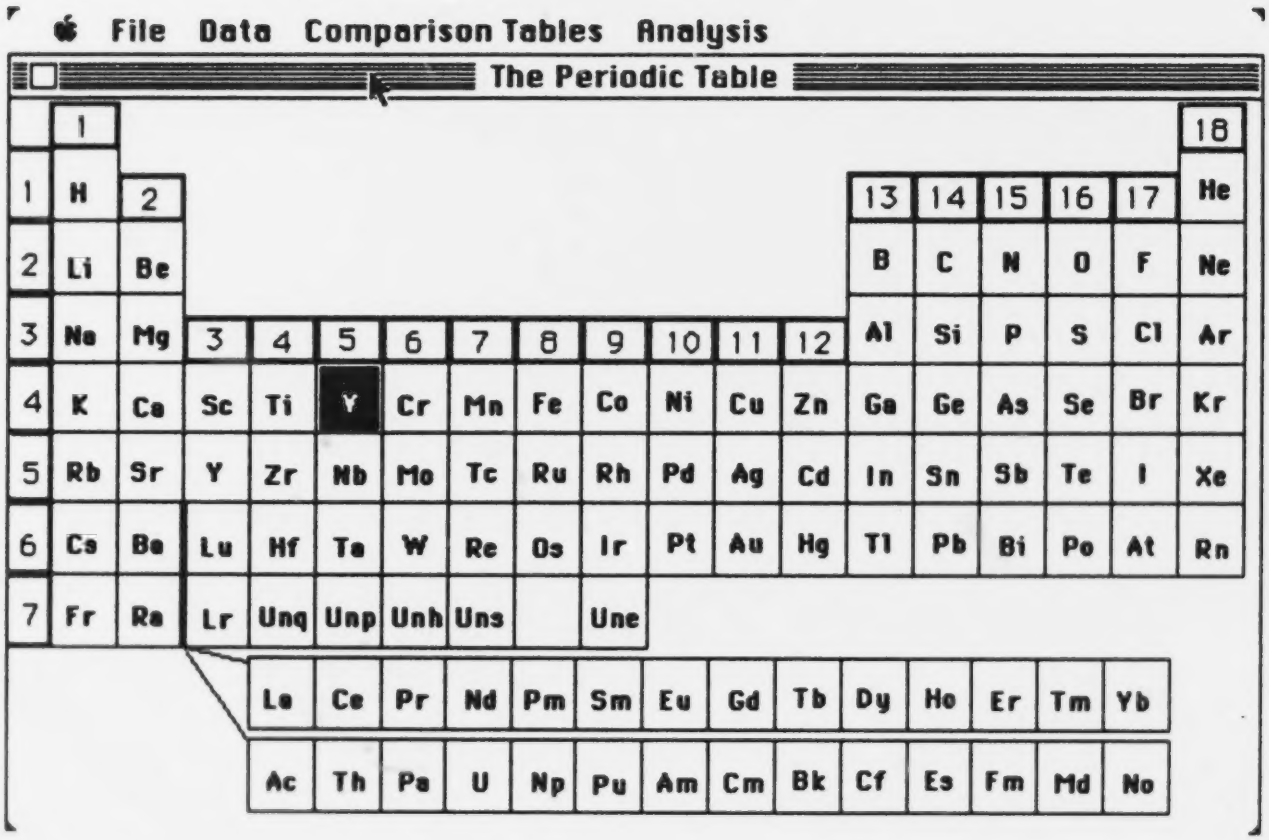

File Data Comparison Tables Analysis
The Periodic Table
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
1 H He
2 Li Be B C N O F Ne
3 Na Mg Al Si P S Cl Ar
4 K Ca Sc Ti Y Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
5 Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
6 Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
7 Fr Ra Lr Unq Unp Unh Uns Une
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No

Fig. 6a. The First Screen of Peri-Chart Showing the Selection of Vanadium (V).

R,S-Stereochemical Designations (Mac with Macstereo), P. A. Wade. Designation of enantiomers is a subject presented in our organic chemistry sequence. Students have a great deal of difficulty visualizing the stereochemical manipulations needed to assign the correct designations. An original program designed to teach this material by presenting demonstrations *and* by testing students on what they have learned was developed in this department. The program, developed on the Lisa, includes worked examples, help messages, and problems for the student to complete. Graphics (See Figure 7) accompany all examples and problems. Students have found Macstereo to be a valuable addition to the traditional use of textbook with models.

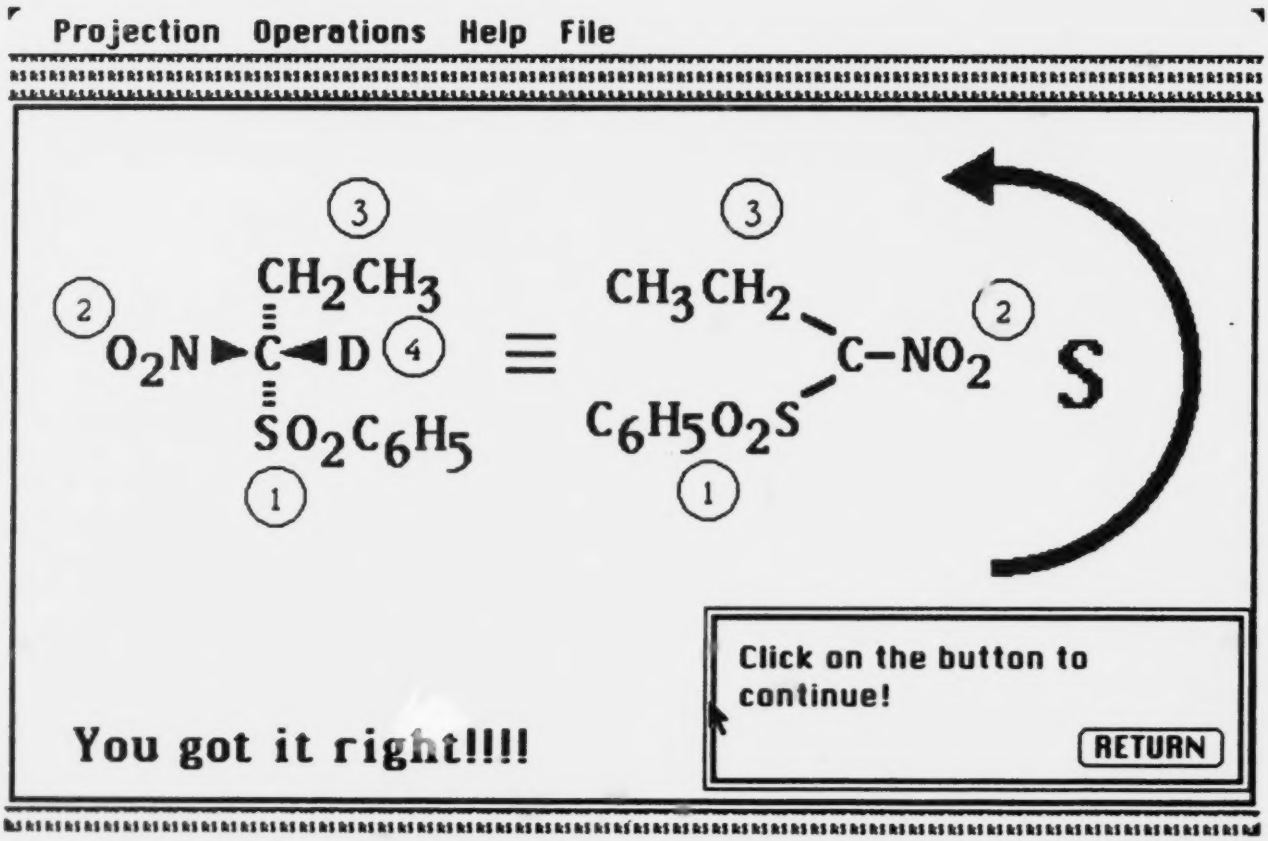


Fig. 7. Problem Created with Macstereo

Computer -Based Molecular Models(Mac with MEC. Molecular Editor and Compiler). A. Smith. Molecular models can be very useful in getting across two basic concepts in molecular structure, shape and atomic "connectivity". Model sets used to help students view systems in three dimensions have limitations. They can handle only relatively small molecules, they require a lot of space to store, and they cannot be used to measure bond lengths. Using MEC, a ball-and-stick molecular model can be rotated in three dimensions.. The screen image of the molecule can be edited by exchanging one atom for another or by deleting atoms or bonds. A number of molecules and crystals have been built including the diamond lattice shown in Figure 8. Distances between atoms can readily be displayed (in Ångstroms) even if there is no bond connecting the atoms, a distinct advantage over conventional model sets. Reaction mechanisms such as Walden inversions and the chair-boat conformational change in cyclohexane can be viewed in three dimensions.

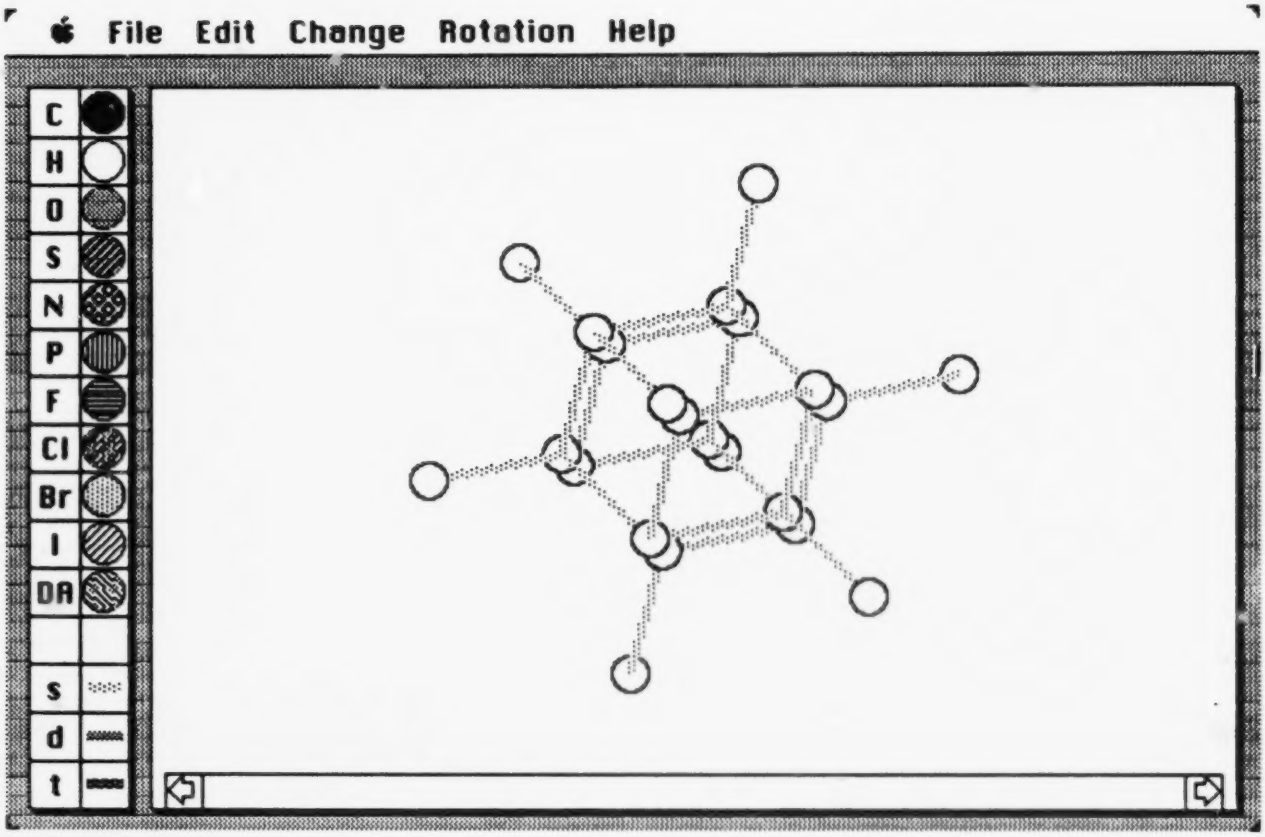
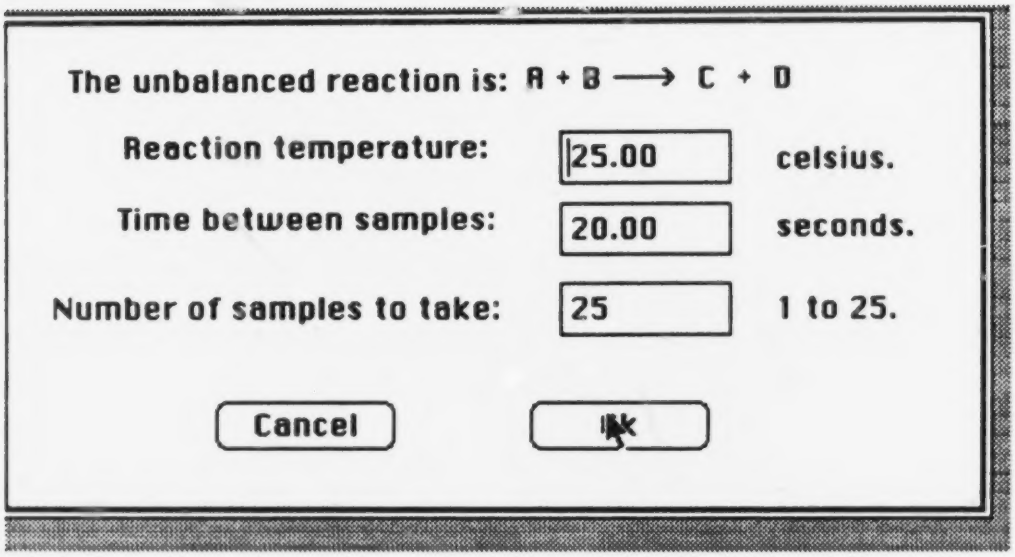


Figure 8. A View of the Diamond Lattice

Simulations

Kinetics Simulations (Mac with KSIMS). A. Smith, R. Inaker. In their laboratory classes students have the opportunity to determine the rate laws for one or two chemical reactions at room temperature. Using the KSIMS program students can run many different kinds of reactions under a variety of conditions. For instance, the student may choose a reaction and vary the concentrations of reactants, the intervals between sampling, and the temperature. The results of each simulated experiment are plotted within seconds using the plotting program built into the application. (See Figure 9). Students may elect to plot any reactant or product using one of several possible plotting funtions in their attempt to determine the rate law of their reaction. This ability to vary the parameters and the resulting plots allows a great deal of information to be examined in a very short period of time. Five years ago, when we first introduced this simulation into general chemistry, we used the KSIMS solftware available from CONDUIT on a Prime computer. The Macintosh version of KSIMS is completed and is now being used in our freshman chemistry course. KSIMS assignments have also been given in a graduate course in chemical kinetics.



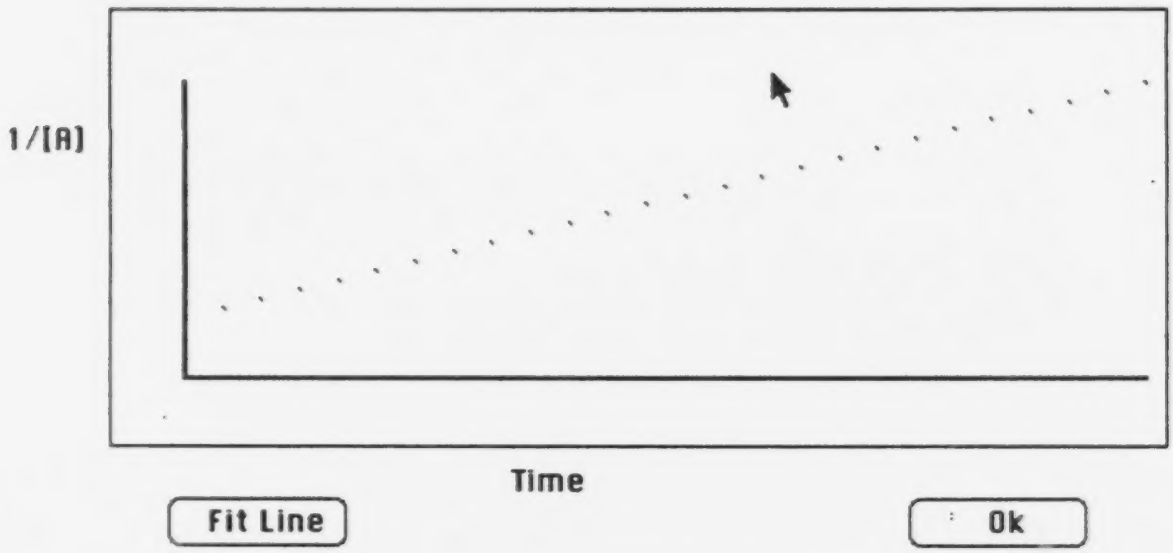
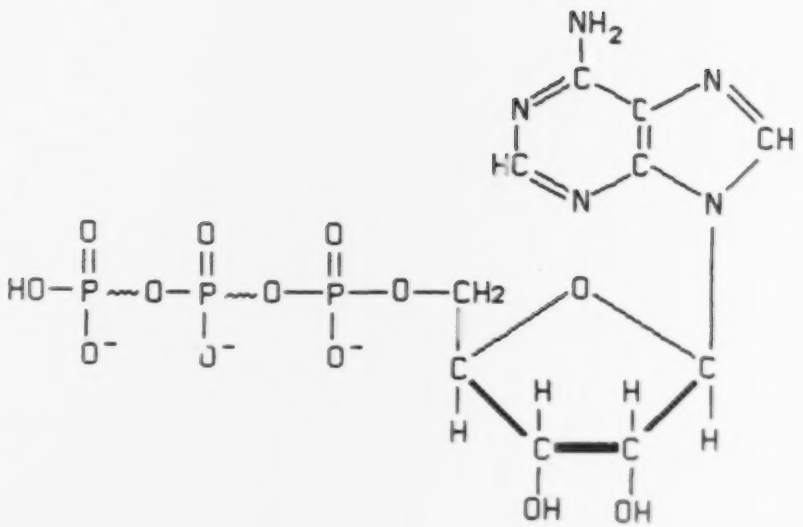


Figure 9. A Kinetic Study (using KSIMS)

Special Assignments

Creating 2-Dimensional models (Mac with MacPaint) Students are asked to design their own "model sets" by constructing the appropriate fragments and combining them into more complex molecules. (See Figure 10 where segments of nucleic acids were created in this way).

Pamela Sherba
N473-section 4
April 23,1985



ATP (Adenosine Triphosphate)

Figure 10. A Student Assignment

* The **Lesson Writer** is an "application" developed (in the Drexel chemistry department) for the Macintosh that allows the user to write an interactive tutorial lesson. Replies to as many as 30 anticipated student inputs can be specified and graphics can be included. No special programming skills are required to create lessons in this way. The **Lesson Writer** is designed to make use of the same techniques involved in producing **MacWrite** and **MacPaint** documents. Special features allow the user to specify whether or not typed spaces are to be omitted or whether lower case letters should be distinguished from upper case letters. Questions can be scored. Students can be branched from one question to another depending upon their performance. Hints ("little" and"big") can be provided. Another related application called **Lesson Runner** is distributed to students. The **Lesson Runner** allows lessons to be run, but not written.

Conclusion

Within the past year we have introduced most of the above computer aided instructional (CAI) materials into our chemistry curriculuum. Nearly all students surveyed indicated that the computer materials made topics treated easier to learn and more fun to study. In the next year we plan to conduct a variety of controlled experiments to see how effective these materials are and to find ways to improve them.